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14. ABSTRACT
We study a scalable, parallel mechanism for stochastic identification/control for problems constrained by PDEs with random input data. Several identification objectives are discussed that either minimize the expectation of a tracking cost functional or minimize the difference of desired statistical quantities in the appropriate L^p norm, and the distributed parameters/control can both deterministic or stochastic. The modeling process may describe the solution in terms of high dimensional spaces, particularly in the case when the input data (coefficients, forcing terms, boundary conditions, geometry, etc) are affected by a large amount of uncertainty. For higher accuracy, the computer simulation must increase the number of random variables (dimensions), and expend more effort approximating the QoI in each individual dimension. We introduce a novel stochastic parameter identification algorithm that integrates an adjoint-based deterministic algorithm with the sparse grid stochastic collocation FEM approach. This allows for decoupled, moderately high dimensional, parameterized computations of the stochastic optimality system and optimal identification of statistical moments (mean value, variance, covariance, etc.) or even the whole probability distribution of system responses.

15. SUBJECT TERMS
uncertainty quantification, stochastic collocation, optimal control, parameter identification, partial differential equations

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EFFICIENT NUMERICAL APPROXIMATIONS AND TRACKING OF STATISTICAL QUANTITIES OF INTEREST FROM THE SOLUTION OF HIGH DIMENSIONAL STOCHASTIC PARTIAL DIFFERENTIAL EQUATIONS

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Abstract

Mathematical modeling and computer simulations are nowadays widely used tools to predict the behavior of problems in engineering and in the natural and social sciences. All such predictions are obtained by formulating mathematical models and then using computational methods to solve the corresponding problems. We use a probability theory approach for *uncertainty quantification* (UQ) since it is particularly well suited for SPDE models, and focus on the broad research areas of algorithmic development and numerical analysis for the discretization of systems of linear or nonlinear SPDEs, building upon and significantly extending our previous successful work.

We conduct comprehensive theoretical and computational comparison of the efficiency, accuracy, and range of applicability of *non-intrusive* methods, such as stochastic collocation methods, and *intrusive* techniques, such as stochastic Galerkin methods, for solving SPDEs and for UQ applications.

We extend the algorithmic and analysis advances wrought by these efforts to the even more challenging settings of optimal control and parameter identification problems for SPDEs. The parameter identification problem is especially important in the SPDE setting since it provides a very useful mechanism for determining statistical information about the input parameters from, e.g., measurements of output quantities. This effort builds on our previous work on adjoint and sensitivity-based methods for deterministic optimal control and parameter identification problems to develop similar methods for tracking statistical quantities of interest from the computational solutions of linear and nonlinear SPDEs driven by high-dimensional random inputs.

Status/Progress

1. **A generalized methodology for the solution of stochastic identification problems constrained by partial differential equations with random input data** [5]
   We propose and analyze a scalable, parallel mechanism for stochastic identification/control for problems constrained by partial differential equations with random input data. Several identification objectives are discussed that either minimize the expectation of a tracking cost functional or minimize the difference of desired statistical quantities in the appropriate L^p norm, and the distributed parameters/control can both deterministic or stochastic. Given an objective we prove the existence of an optimal solution, establish the validity of the Lagrange multiplier rule and obtain a stochastic optimality system of equations. The modeling process may describe the solution in terms of high dimensional spaces, particularly in the case when the input data (coefficients, forcing terms, boundary conditions, geometry, etc) are affected by a large amount of uncertainty. For higher accuracy, the computer simulation must increase the number of random variables (dimensions), and expend more effort approximating the quantity of interest in each individual dimension. Hence, we introduce a novel stochastic parameter identification algorithm that integrates an adjoint-based deterministic algorithm with the sparse grid stochastic collocation FEM

approach. This allows for decoupled, moderately high dimensional, parameterized computations of the stochastic optimality system, where at each collocation point, deterministic analysis and techniques can be utilized. The advantage of our approach is that it allows for the optimal identification of statistical moments (mean value, variance, covariance, etc.) or even the whole probability distribution of the input random fields, given the probability distribution of some responses of the system (quantities of physical interest). Our rigorously derived error estimates, for the fully discrete problems, will be described and used to compare the efficiency of the method with several other techniques. Numerical examples illustrate the theoretical results and demonstrate the distinctions between the various stochastic identification objectives.

The general framework of the problem is the following: we seek random parameters, coefficients $\kappa(\omega, x)$ and/or forcing terms $f(\omega, x)$, with $x \in D \subset \mathbb{R}^d$, $\omega \in \Omega$, where $(\Omega, \mathcal{F}, P)$ a complete probability space, that minimize the mismatch between stochastic measured and simulated data. Here Ω is the set of outcomes, $\mathcal{F} \subset 2^\Omega$ is the σ-algebra of events and $P : \mathcal{F} \to [0, 1]$ is a probability measure. There are two main ways of measuring this spatial-stochastic quantity: the expected value of spatial mismatch (see e.g. [8, 7] more ref's) and the spatial mismatch of averages of the statistical quantities of interest. More precisely, we consider the minimization cost functionals of the type

$$\mathcal{J}(u, (\kappa, f)) \tag{0.1}$$

over all κ,f and random solutions $u : \Omega \times \overline{D} \to \mathbb{R}$ that satisfy P-almost everywhere in Ω, or in other words almost surely (a.s.), the following stochastic boundary value problem:

$$\mathcal{L}(\kappa)(u) = f \quad \text{in } D \tag{0.2}$$

supplemented with appropriate boundary conditions.

We consider the groundwater flow problem in a region $D \subset \mathbb{R}^d$, $d = 1, 2, 3$, where the flux is related to the hydraulic head gradient by Darcy's law. We model the uncertainties in the soil by describing the conductivity coefficient κ as a random field denoted $\kappa(\omega, x)$. Similarly, the stochastic forcing term $f(\omega, x)$ models the uncertainty in the sources and sinks.Therefore the hydraulic head $u : \Omega \times D$ is also a random field satisfying the elliptic stochastic partial differential equation (SPDE):

$$\begin{cases} -\nabla \cdot (\kappa(\omega, x)\nabla u(\omega, x)) = f(\omega, x) & \text{in } \Omega \times D, \\ \qquad\qquad u = 0 & \text{on } \Omega \times \partial D. \end{cases} \tag{0.3}$$

The linear elliptic SPDE (0.3) with $\kappa(\omega, \cdot)$ uniformly bounded and coercive, i.e.

$$\text{there exists } \kappa_{min}, \kappa_{max} \in (0, +\infty) \text{ such that } P(\omega \in \Omega : \ \kappa(\omega, x) \in [\kappa_{min}, \kappa_{max}] \, \forall x \in \overline{D}) = 1 \tag{0.4}$$

and $f(\omega, \cdot)$ square integrable with respect to P, satisfies assumptions A_1 and A_2 with $W(D) = H_0^1(D)$. We shall assume that D is a bounded and open subset of $\mathbb{R}^d$, either with smooth boundary (of class C^2 for instance) or convex. This implies that for every $f \in L_P^2(\Omega; L^2(D))$, problem (0.3) has a unique solution $u \in L_P^2(\Omega; H_0^1(D) \cap H^2(D))$. The solution to (0.3) must be understood in a variational sense, i.e., for given $f \in L_P^2(\Omega, L^2(D))$ we say that $u \in L_P^2(\Omega, H_0^1(D))$ is a solution of

$$\mathbb{E}\left[\int_D \sum_{i=1}^{d} \kappa(\cdot, x)\partial_{x_i} u(\cdot, x)\partial_{x_i} z(x) - f(\cdot, x)z(x)dx\right] = 0, \quad \forall z \in H_0^1(D). \tag{0.5}$$

To simplify the presentation, we use operator $\mathcal{L}$ to represent the Poisson operator introduce in forward state equation (0.3). Here we need to introduce all the admissible sets to simplify the notation going forward. First we define the admissible set of conductivity coefficients given by

$$\mathcal{A}_{ad} = \{\kappa \in L^\infty(\Omega; L^\infty(D)) \mid \kappa(\omega, x) \text{ satisfies (0.4)}\}, \tag{0.6}$$

then given $\kappa \in \mathcal{A}_{ad}$ let the admissible set of states and controls be defined as

$$\mathcal{B}_{ad} = \left\{ (u,f) \mid u \in L^2_P(\Omega; H^1_0(D) \cap H^2(D)) \text{ and } f \in L^2_P(\Omega; L^2(D)) \right\}. \tag{0.7}$$

Finally, given $f \in L^2_P(\Omega; L^2(D))$ let the the admissible set of states and coefficients be described as

$$\mathcal{C}_{ad} = \left\{ (u,\kappa) \mid u \in L^2_P(\Omega; H^1_0(D) \cap H^2(D)) \text{ and } \kappa \in \mathcal{A}_{ad} \right\}. \tag{0.8}$$

We also introduce a stochastic target function $\overline{u} \in L^2_P(\Omega; L^2(D))$, a given possible perturbed observation. We consider a general class of minimization problems for solving the stochastic inverse problem for the random forcing function $f(\omega, x)$ and the solution $u(\omega, x)$ satisfying a.s. (0.3). Here we assume given the input random process $\kappa \in \mathcal{A}_{ad}$ and the target $\overline{u} \in L^2_P(\Omega; L^2(D))$ and we want to recover (u^*_J, f^*_J) such that

$$(u^*_J, f^*_J) = \inf_{(u,f)\in\mathcal{B}_{ad}} \{J(u,f) : \text{ subject to (0.3)}\} \tag{0.9}$$

where $J(u,f)$ is a given stochastic functional constructed to track the desired random fields or the statistical quantities of interest (QoI) of such stochastic functions. This leads to the following definition. A pair $(u^*_J, f^*_J) \in \mathcal{B}_{ad}$ satisfying (0.3) a.s., for which the infimum in (0.9) is attained are called the *stochastic optimal pair* and the control $\widetilde{f}$ is referred as *stochastic optimal control*. In what follows we will describe two functionals, denoted $J_1(u,f)$ and $J_2(u,f)$ used to solve stochastic optimal control problems. The first, described by (0.10), is based on the standard classical approach based on stochastic least squares approximation whereas the second, described by (0.14), uses statistical tracking objectives and is easily generalized. We will also describe the corresponding adjoint equations, optimality conditions and state the necessary conditions for existence and uniqueness of the stochastic optimal pair.

The optimal control problem using stochastic least squares minimization

For $\kappa \in \mathcal{A}_{ad}$ given data, we consider the following optimal control problem associated with a stochastic elliptic boundary value problem:

$$\text{(P.1)} \quad \begin{cases} \textit{Minimize the cost functional} \\[2ex] J_1(u,f) = \mathbb{E}\left[\dfrac{1}{2}\|u(\omega,\cdot) - \overline{u}(\omega,\cdot)\|^2_{L^2(D)} + \dfrac{\alpha}{2}\|f(\omega,\cdot)\|^2_{L^2(D)}\right], \\[2ex] \textit{on all } (u,f) \in \mathcal{B}_{ad} \textit{ subject to the stochastic state equations (0.3).} \end{cases} \tag{0.10}$$

Using standard techniques (see e.g. [13, 14, 1, 2, 15, 10, 9, 7]) one can prove that the problem (0.10)-(0.3) has a unique optimal pair that is characterized by a maximum principle type result.

$(\widehat{u}, \widehat{f})$ is the unique optimal pair in problem (0.10)-(0.3) if and only if there exists $\xi \in L^2_P(\Omega; H^1_0(D))$ such that

$$\begin{aligned} -\nabla\cdot(\kappa(\omega,x)\nabla\xi(\omega,x)) &= \widehat{u}(\omega,x) - \overline{u}(\omega,x) \quad && \textit{a.e. in } \Omega\times D, \\ \xi(\omega,x) &= 0 && \textit{a.e. in } \Omega\times\partial D. \end{aligned} \tag{0.11}$$

and

$$\widehat{f}(\omega,x) = -\frac{1}{\alpha}\,\xi(\omega,x) \qquad \textit{a.e. in } \Omega\times D. \tag{0.12}$$

Therefore the solution of the control problem is the solution of the *optimality* system:

$$\begin{array}{llll} \text{(the state equations)} & -\nabla\cdot(\kappa\nabla\widehat{u}) = \widehat{f} & \text{in } \Omega\times D, & \text{and } u = 0 \text{ in } \Omega\times\partial D; \\ \text{(the adjoint equations)} & -\nabla\cdot(\kappa\nabla\xi) = \widehat{u} - \overline{u} & \text{in } \Omega\times D, & \text{and } \xi = 0 \text{ in } \Omega\times\partial D. \\ \text{(and the optimality condition)} & \widehat{f} = -\frac{1}{\alpha}\xi & \text{a.e. in } \Omega\times D. & \end{array} \tag{0.13}$$

The necessary and sufficient conditions (0.13) are a system of *coupled* stochastic partial differential equations whose solution yields the optimal control $\widehat{f}$, the optimal state $\widehat{u}$ and the optimal adjoint state ξ.

The optimal control problem utilizing statistical tracking objectives

Now we aim at matching expected values, i.e., we consider the following problem:

$$\text{(P.2)} \quad \begin{cases} \textit{Minimize the cost functional} \\ J_2(u,f) = \dfrac{1}{2}\displaystyle\int_D \big[\mathbb{E}u(\cdot,x) - \mathbb{E}\overline{u}(\cdot,x)\big]^2 dx + \dfrac{\alpha}{2}\int_D \mathbb{E}f^2(\cdot,x)dx, \\ \textit{on all } (u,f) \in \mathcal{B}_{ad} \textit{ subject to the stochastic state equations } (0.3). \end{cases} \tag{0.14}$$

Note that

$$\int_D \big[\mathbb{E}u(\cdot,x) - \mathbb{E}\overline{u}(\cdot,x)\big]^2 dx \le \mathbb{E}\Big(\|u-\overline{u}\|^2_{L^2(D)}\Big),$$

which justifies the functional (0.14).

$(\widetilde{u},\widetilde{f})$ is the optimal pair in problem (0.10),(0.3) if and only if there exists $\xi \in L^2_P(\Omega; H^1_0(D))$ such that

$$\begin{aligned} -\nabla\cdot(\kappa(\omega,x)\nabla\xi(\omega,x)) &= \mathbb{E}\big(\widetilde{u}(\cdot,x) - \overline{u}(\cdot,x)\big) && \textit{in } \Omega\times D, \\ \xi(\omega,x) &= 0 && \textit{in } \Omega\times\partial D. \end{aligned} \tag{0.15}$$

and

$$\widetilde{f}(\omega,x) = -\frac{1}{\alpha}\,\xi(\omega,x) \qquad \textit{a.e. in } \Omega\times D. \tag{0.16}$$

Therefore the solutions of the control problem are the solutions of the *optimality* system:

$$\begin{array}{llll} \text{(the state equations)} & -\nabla\cdot(\kappa\nabla\widetilde{u}) = \widetilde{f} & \text{in } \Omega\times D, & \text{and } u=0 \text{ in } \Omega\times\partial D, \\ \text{(the adjoint equations)} & -\nabla\cdot(\kappa\nabla\xi) = \mathbb{E}(\widetilde{u}-\overline{u}) & \text{in } \Omega\times D, & \text{and } \xi=0 \text{ in } \Omega\times\partial D, \\ \text{(and the optimality condition)} & \widetilde{f} = -\frac{1}{\alpha}\xi & \text{a.e. in } \Omega\times D. & \end{array} \tag{0.17}$$

The conditions (0.17) resemble the optimality system (0.13), the difference is only in the adjoint equation which has a deterministic right-hand side. Nevertheless, the adjoint variable is still a stochastic quantity, the adjoint operator having stochastic coefficients.

Stochastic parameter identification problems

We also study the identification of the coefficient κ in the stochastic boundary value problem (0.3). In the deterministic case, the direct problem, where κ is given, the existence and uniqueness results are well known, see e.g. [11]. The linear deterministic inverse problem related to (0.3) has been studied in e.g. [1], for the nonlinear deterministic see e.g. [3].

For the identification problem, we are given a possible perturbed observation $\overline{u}$ corresponding to the state variable u and we must determine κ in (0.3) such that $u(\kappa) = \overline{u}$ in $\Omega\times D$. Of course, such an κ may not exist.

Parameter identification using stochastic least squares minimization

The least squares approach leads us to the minimization problem:

$$\text{(P.3)} \quad \begin{cases} \textit{Minimize the cost functional} \\ J_3(u,\kappa) = \mathbb{E}\left[\frac{1}{2}\|u-\overline{u}\|^2_{L^2(D)} + \frac{\beta}{2}\|\kappa\|^2_{L^2(D)}\right], \\ \textit{on all } (u,\kappa)\in\mathcal{C}_{ad} \textit{ subject to the stochastic state equations } (0.3). \end{cases} \tag{0.18}$$

Let (u^*,κ^*) be an optimal pair in problem (0.3) and (0.18). Then

$$\kappa^*(\omega,x) = \max\{\kappa_{\min}, \min\{\frac{1}{\beta}\nabla u^*(\omega,x)\nabla\eta(\omega,x), \kappa_{\max}\}\} \quad a.e. \ in \ \Omega\times D \tag{0.19}$$

where $\eta\in L^2_P(\Omega;H^1_0(D))$ is the solution of

$$\begin{aligned} -\nabla\cdot(\kappa^*(\omega,x)\nabla\eta(\omega,x)) &= u^*(\omega,x)-\overline{u}(\omega,x) \quad && in\ \Omega\times D, \\ \eta(\omega,x) &= 0 && in\ \Omega\times\partial D. \end{aligned} \tag{0.20}$$

Parameter identification utilizing statistical tracking objectives
For the identification problem matching expected values, given a possible perturbed observation $\overline{u}$ corresponding to the state variable u, we seek κ in (0.3) such that $\mathbb{E}u(\kappa)=\mathbb{E}\overline{u}$ in D. Therefore we consider the problem:

$$\text{(P.4)} \quad \begin{cases} \textit{Minimize the cost functional} \\ J_4(u,\kappa) = \frac{1}{2}\int_D \left[\mathbb{E}u(\cdot,x)-\mathbb{E}\overline{u}(\cdot,x)\right]^2 dx + \frac{\beta}{2}\int_D \mathbb{E}\kappa^2(\cdot,x)dx, \\ \textit{on all } (u,\kappa)\in\mathcal{C}_{ad} \textit{ subject to the stochastic state equations } (0.3). \end{cases} \tag{0.21}$$

Let $(\mathring{u},\mathring{\kappa})$ be an optimal pair in problem (0.3) and (0.21). Then

$$\mathring{\kappa}(\omega,x) = \max\{\kappa_{\min}, \min\{\frac{1}{\beta}\nabla\mathring{u}(\omega,x)\nabla\eta(\omega,x), \kappa_{\max}\}\} \quad a.e. \ in \ \Omega\times D \tag{0.22}$$

where $\eta\in L^2_P(\Omega;H^1_0(D))$ is the solution of

$$\begin{aligned} -\nabla\cdot(\mathring{\kappa}(\omega,x)\nabla\eta(\omega,x)) &= \mathbb{E}\big(\mathring{u}(\cdot,x)-\overline{u}(\cdot,x)\big) \quad && in\ \Omega\times D, \\ \eta(\omega,x) &= 0 && in\ \Omega\times\partial D. \end{aligned} \tag{0.23}$$

Identification of higher order moments
If one is interested in matching covariance, and/or higher order moments, the cost functional used in problem (0.21) can be generalized as follows. Assume we are interested in $\mathcal{L}$-order moments, and $f\in L^{\mathcal{L}}_P(\Omega;L^{2\mathcal{L}-2}(D))$ then

$$\text{(P.5)} \quad \begin{cases} \textit{Minimize the cost functional} \\ J_5(u,\kappa) = \sum_{\ell=1}^{\mathcal{L}}\frac{1}{2\ell}\int_D \left[\mathbb{E}u^\ell(\cdot,x)-\mathbb{E}\overline{u}^\ell(\cdot,x)\right]^2 dx + \frac{\beta}{2}\int_D \mathbb{E}\kappa^2(\cdot,x)dx, \\ \textit{on all } (u,\kappa)\in\mathcal{C}_{ad} \textit{ subject to the stochastic state equations } (0.3). \end{cases} \tag{0.24}$$

Let $(\mathring{u}, \mathring{\kappa})$ be an optimal pair in problem (0.3) and (0.24). Then

$$\mathring{\kappa}(\omega, x) = \max\{\kappa_{\min}, \min\{\frac{1}{\beta}\nabla\mathring{u}(\omega, x)\nabla\eta(\omega, x), \kappa_{\max}\}\} \quad a.e. \ in \ \Omega \times D \tag{0.25}$$

where $\eta \in L_P^{\mathcal{L}}(\Omega; H_0^1(D) \cap L^{2\mathcal{L}}(D))$ is the solution of

$$\begin{aligned} -\nabla \cdot (\mathring{\kappa}(\omega, x)\nabla\eta(\omega, x)) \ &= \sum_{\ell=1}^{\mathcal{L}} \mathring{u}^{\ell-1}\mathbb{E}\big(\mathring{u}^{\ell}(\cdot, x) - \overline{u}^{\ell}(\cdot, x)\big) \quad && in \ \Omega \times D, \\ \eta(\omega, x) \ &= 0 && in \ \Omega \times \partial D. \end{aligned} \tag{0.26}$$

We illustrate the convergence of the generalized stochastic collocation (gSC), for identifying the random process $\kappa(\omega, x)$ coming from the solution of the stochastic linear elliptic problem described in 0.3, in one spatial dimension. We will exemplify the algorithm using both the expected value of spatial mismatch and the spatial mismatch of averages of the statistical quantities of interest. The rates of convergence are derived from estimates of the forward problem and the computational results are in accordance with the convergence rates predicted by the theory. However, for matching the expected value of the parameter and the state, *we observe faster convergence when employing the statistical tracking objective than the standard stochastic least squares minimization, which suggests the inclusion of higher order moments to the tracking functionals may result in even better statistical description of random fields.*
Finally, we will also use this problem to compare the convergence of the gSC approach with Monte Carlo methods for solving the stochastic optimality system resulting from the stochastic parameter identification approach, see Table 0.1. Given a stochastic target $\overline{u}(\omega, x)$ and random process $f(\omega, x)$ the problem is to identify the optimal coefficient $\kappa_J^*(\omega, x)$ and state $u_J^*(\omega, x)$ satisfying

$$J(u_J^*, \kappa_J^*) = \inf_{(u,\kappa)\in\mathcal{C}_{ad}} J(u, \kappa), \tag{0.27}$$

subject to

$$\begin{cases} -\nabla \cdot (\kappa(\omega, \cdot)\nabla u(\omega, \cdot)) &= f(\omega, \cdot) \quad \text{in } \Omega \times D, \\ u(\omega, \cdot) &= 0 \quad \text{on } \Omega \times \partial D, \end{cases} \tag{0.28}$$

with $D = [0, 1]$. For this example we will consider both identification problems by letting $J = J_3$ and $J = J_4$ described by equations (0.18) and (0.21). For both optimization problems we assume we are given the exact stochastic target, described as

$$\overline{u}(\omega, x) = x(1 - x^2) + \sum_{n=1}^{N} \sin\left(\frac{n\pi x}{L_u}\right) Y_n(\omega), \tag{0.29}$$

and we want the desired optimal (true) random coefficient $\overline{\kappa}$ to be given by

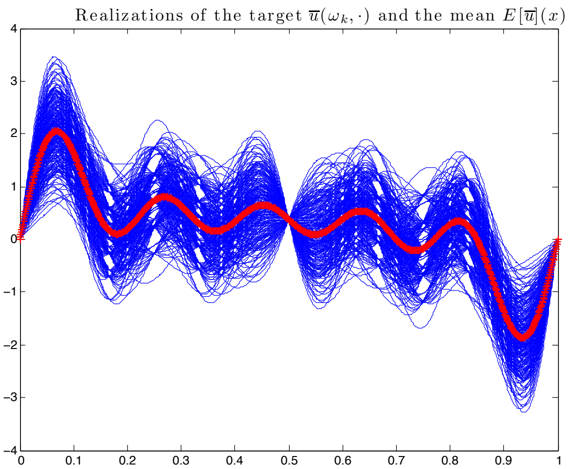
$$\overline{\kappa}(\omega, x) = (1 + x^3) + \sum_{n=1}^{N} \cos\left(\frac{n\pi x}{L_\kappa}\right) Y_n(\omega). \tag{0.30}$$

The goal of computation will be to find the optimal $(\kappa_{J_3}^*, u_{J_3}^*)$ and $(\kappa_{J_4}^*, u_{J_4}^*)$ that satisfy (0.27) - (0.28) with a given fixed stochastic load defined as the exact right-hand, i.e.,

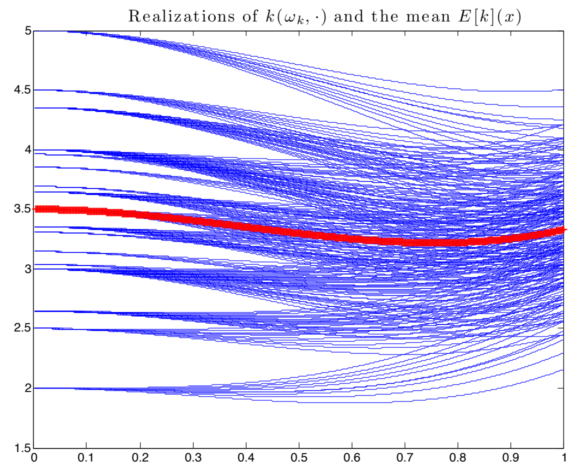
$$f(\omega, x) = -\nabla \cdot (\overline{\kappa}(\omega, x)\nabla\overline{u}(\omega, x)). \tag{0.31}$$

For $x \in D$ we let $L_u = 2N$ and $L_\kappa = 1/2$ and we note that both random expressions for $\overline{u}$ and $\overline{\kappa}$ are related to a truncated Karhunen-Loève expansion of a one-dimensional stationary covariance. However, this is just a test problem where we have guaranteed well-posedness through the construction of an uniformly

bounded and coercive $\kappa(\omega, x)$ and enforced isotropy when assembling the random target $\overline{u}$, the stochastic process $\overline{\kappa}(\omega, x)$ to be identified and forcing function $f(\omega, x)$ with respect to the random domain Γ^N. In this example, all the random variables $\{Y_n(\omega)\}_{n=1}^N$ are independent, have zero mean and unit variance, i.e. $\mathbb{E}[Y_n] = 0$ and $\mathbb{E}[Y_n Y_m] = \delta_{nm}$ for $n, m \in \mathbb{N}_+$, and are uniformly distributed in the interval $[0, 1]$.
We combine the gSC approximations with an gradient-based optimization method, for solving (0.27) - (0.28). First, we plot several ensembles, sampled from the Clenshaw-Curtis sparse grid $\mathscr{H}(3, 5)$, of the target $\overline{u}(\mathbf{Y}(\omega_k), x)$, the the exact input parameter $\overline{\kappa}(\mathbf{Y}(\omega_k), x)$ and the right-hand side $f(\mathbf{Y}(\omega_k), x)$, for $k = 1, \dots, M = 241$, and the corresponding expected values $\mathbb{E}[\overline{u}](x)$, $\mathbb{E}[\overline{\kappa}](x)$ and $\mathbb{E}[f](x)$ in Figures 0.1(a), 0.1(b) and 0.1(c) respectively. The finite element space for the spatial discretization is the span of continuous functions that are piecewise polynomials with degree two over a uniform partition of D with 1225 unknowns.



(a)



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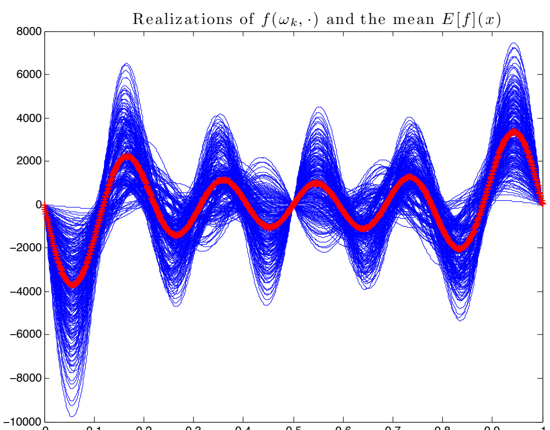


(c)

Fig. 0.1: For a finite dimensional probability space Γ^N, with $N = 5$ we plot $k = 1, \dots, M = 241$ realizations (*blue*), corresponding to Clenshaw-Curtis samples from the isotropic sparse grid $\mathscr{H}(3, 5)$, and the exact expectation (*red*) of: (1) the stochastic target $\overline{u}(\omega, x)$, (2) the true input parameter $\overline{\kappa}(\omega, x)$ and (3) the forcing function $f(\omega, x)$.

Instead of solving the optimality systems, a gradient algorithm is used to design the optimal stochastic coefficient $\kappa^*_{J_3}(\omega, x)$ and $\kappa^*_{J_4}(\omega, x)$ respectively. The first step involves computing the gradient of the cost

functionals $\frac{d}{d\kappa}J_3(u,\kappa)$ and $\frac{d}{d\kappa}J_4(u,\kappa)$. In this example the gradient of the cost functionals are evaluated and used in simple minimization framework to estimate the optimal input parameter $\kappa(\omega,x)$. Given the stochastic load f and the target $\overline{u}$, this procedure is described below.

1. Define the number of desired sparse grid collocation points M in Γ^N with the corresponding interpolating basis functions $\{\psi_k(\mathbf{y})\}_{k=1}^M$ of $\mathcal{P}_{\mathbf{p}}(\Gamma^N)$.
2. Set the gradient iteration count $i=0$ and select an initial guess for the input coefficient $\kappa^{(0)}(\mathbf{y},x)$. Set the initial step size $\epsilon<1$ used by the gradient algorithm.
3. Solve the forward problem given by (0.28) using $\kappa^{(i)}$ and construct the corresponding random solution $u|_{\kappa^{(i)}}$.
4. Compute the cost functionals $J_n^{(i)}$, where $n=3,4$ when solving problems (P.3) or (P.4) respectively.
5. Compute the gradient of the cost functionals $\frac{d}{d\kappa}J_n^{(i)}$ where $n=3,4$.
6. Compute an updated random coefficient $\kappa^{(i+1)}=\kappa^{(i)}-\epsilon\frac{d}{d\kappa}J_n^{(i)}$, check the convergence criteria and update the gradient step (if necessary):

For our particular problem described by (0.27) - (0.28) we define the penalty term $\beta=10^{-6}$ for both functionals J_3 and J_4 described by (0.18) and (0.21) respectively. The remaining parameters required by the gradient algorithm are defined as: the initial step size $\epsilon=10^{-3}$, the convergence tolerance $tol=\beta$ and the maximum number of gradient iterations $itermax=10^3$.

The first exhibition of the improvements offered by utilizing out proposed functional J_4 as opposed to J_3 for constructing the optimal pair (u^*,κ^*) can be observed in Figure 0.2.

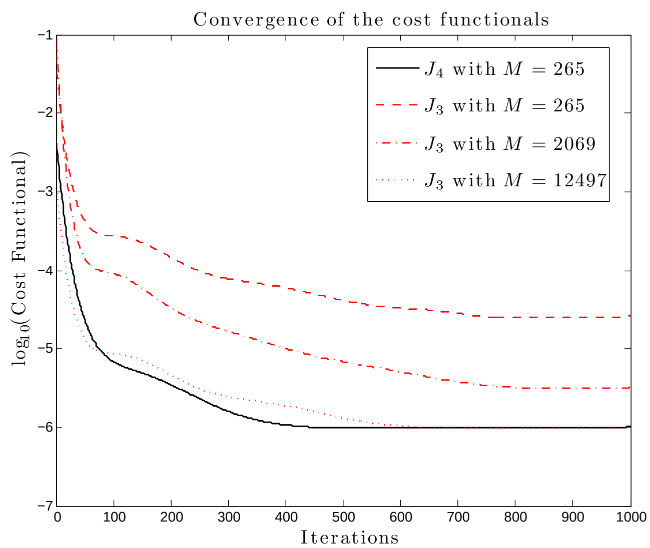
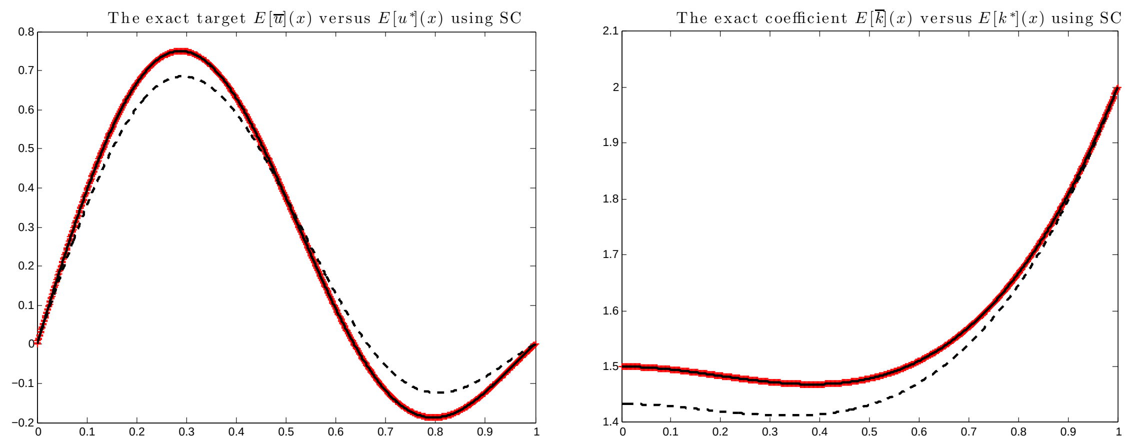


Fig. 0.2: A $N=11$ dimensional comparison of the convergence of cost functionals J_3 and J_4, given by (0.18) and (0.21) respectively, when using the gradient-based sparse grid stochastic collocation method for solving the optimization problem (0.27) - (0.28) with $\beta=10^{-6}$.

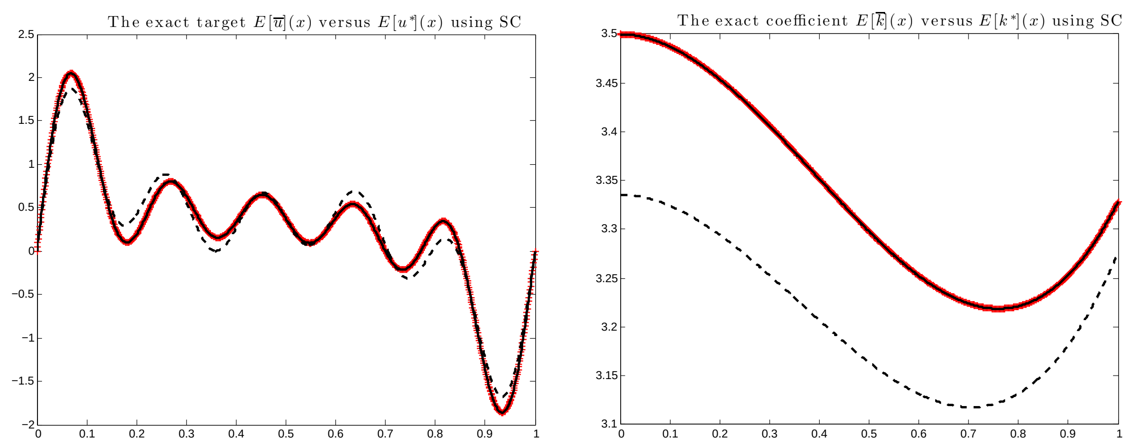
2. **Improved accuracy in regularization models of incompressible flow via adaptive nonlinear filtering** [4]

   We study adaptive nonlinear filtering in the Leray regularization model for incompressible, viscous Newtonian flow. The filtering radius is locally adjusted so that resolved flow regions and coherent flow structures are not 'filtered-out', which is a common problem with these types of models. A numerical method is proposed that is unconditionally stable with respect to timestep, and decouples the problem so that the filtering becomes linear at each timestep and is decoupled from the system. Several numerical examples are given that demonstrate the effectiveness of the method.



(a) (b)

Fig. 0.3: A $N = 1$ dimensional comparison of the gradient-based sparse grid stochastic collocation method, with $M = 5$ collocation points, for solving the optimization problem (0.27) - (0.28) with functionals $J = J_3$ (dashed black) and $J = J_4$ (solid black). We plot: 0.3(a) the exact first moment of the target $\mathbb{E}[\overline{u}]$ (red) versus the expected value of the optimal solution $\mathbb{E}[u^*_{J_3}]$ (dashed black) and $\mathbb{E}[u^*_{J_4}]$ (solid black); 0.3(b) the exact first moment of the coefficient $\mathbb{E}[\overline{\kappa}]$ (red) versus the expected value of the optimal coefficients $\mathbb{E}[\kappa^*_{J_3}]$ (dashed black) and $\mathbb{E}[\kappa^*_{J_4}]$ (solid black).

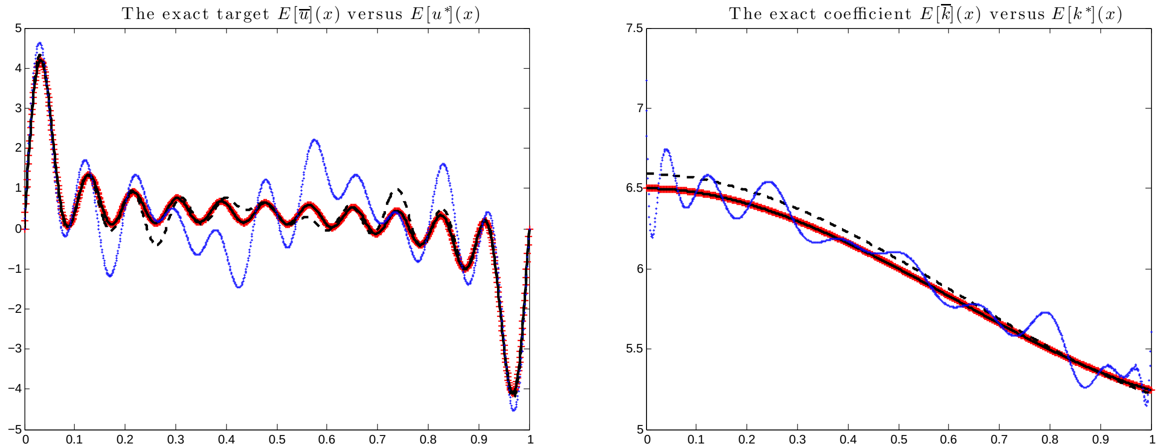


(a) (b)

Fig. 0.4: A $N = 5$ dimensional comparison of a gradient-based sparse grid stochastic collocation method, with $M = 61$ collocation points , for solving the optimization problem (0.27) - (0.28) with functionals $J = J_3$ (dashed black) and $J = J_4$ (solid black). We plot: 0.5(a) the exact first moment of the target $\mathbb{E}[\overline{u}]$ (red) versus the expected value of the optimal solutions $\mathbb{E}[u^*_{J_3}]$ (dashed black) and $\mathbb{E}[u^*_{J_4}]$ (solid black); 0.5(b) the exact first moment of the coefficient $\mathbb{E}[\overline{\kappa}]$ (red) versus the expected value of the optimal coefficients $\mathbb{E}[\kappa^*_{J_3}]$ (dashed black) and $\mathbb{E}[\kappa^*_{J_4}]$ (solid black).

3. **Analysis of stability and errors of IMEX methods for magnetohydrodynamics flows at small Reynolds number** [12]

The MHD flows are governed by the Navier-Stokes equations coupled with the Maxwell equations through



(a) (b)

Fig. 0.5: A $N = 11$ dimensional comparison of a gradient-based sparse grid stochastic collocation (SC) method, using $M = 265$ collocation points with a gradient-based Monte Carlo (MC) method using 1.2×10^6 samples, for solving the optimization problem (0.27) - (0.28). We plot: 0.5(a) the exact first moment of the target $\mathbb{E}[\overline{u}]$ (red) versus the expected value of the optimal solution $\mathbb{E}[u^*_{\mathcal{J}_3}]$ using SC (dashed black), $\mathbb{E}[u^*_{\mathcal{J}_4}]$ using SC (solid black) as well as $\mathbb{E}[u^*_{\mathcal{J}_4}]$ using MC (dotted blue); 0.5(b) the exact first moment of the coefficient $\mathbb{E}[\overline{\kappa}]$ (red) versus the expected value of the optimal coefficient $\mathbb{E}[\kappa^*_{\mathcal{J}_3}]$ using SC (dashed black), $\mathbb{E}[\kappa^*_{\mathcal{J}_4}]$ using SC (solid black) as well as $\mathbb{E}[\kappa^*_{\mathcal{J}_4}]$ using MC (dotted blue).

N	SG	MC
5	61	7e+03
11	1581	9e+06
21	13329	8e+09

Table 0.1: For Γ^N, with $N = 5, 11$ and 21, we compare the number of deterministic solutions required by the sparse grid method (SG) using Clenshaw-Curtis abscissas and the Monte Carlo (MC) method using random abscissas, to reduce the original error in both $\left\|\mathbb{E}[u^*_{\mathcal{J}_4}] - \mathbb{E}[\overline{u}]\right\|_{L^2(D)}$ and $\left\|\mathbb{E}[\kappa^*_{\mathcal{J}_4}] - \mathbb{E}[\overline{\kappa}]\right\|_{L^2(D)}$ by a factor of 10^4.

coupling terms. The physical processes of fluid flows and electricity and magnetism are quite different and non-model problems can require different meshes, time steps and methods. We introduce a implicit-explicit (IMEX) method where the MHD equations can be evolved in time by calls to the NSE and Maxwell codes, each possibly optimized for the subproblem's respective physics.

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Honors & Awards Received

None

AFRL Point of Contact

Transitions

None

New Discoveries

None